

## REMARKS

### *General:*

Claims 1-11 are pending in this application. Claims 5, 8, 9, and 10 are amended in this response. No new matter has been added by this amendment.

### *Title:*

The title was objected to as incorrect, because it referred to a “method and apparatus” whereas the pending claims are all directed to the method. The title is now brought into agreement with the claims by deleting the words “and apparatus.”

### *35 U.S.C. § 101:*

Claims 1-11 were rejected as directed to non-statutory subject matter, namely computational methods without requiring the performance of a physical transformation.

It is respectfully submitted that the process claimed falls within the “Safe Harbor” of MPEP § 2106.IV.B.2.(b).i), second heading (pages 2100-16 and 2100-17 of the Feb. 2003 revision) for “Manipulation of Data Representing Physical Objects,” and thus constitutes statutory subject matter.

The present process starts with measurements of physical objects (the crystal powder from which the diffraction pattern provided at claim 1, line 3 is obtained). The process is directed essentially to processing the data representing the physical crystal (see, for example, claim 1, lines 4 and 13-14). The calculated structure generated at the end of the process has real-world value in enabling the user to identify which of two or more isomers having the same analytical formula the original crystal powder consists of. This is useful because different isomers may have different pharmacological or other chemical properties. After finding experimentally a material with particular properties, identifying the active isomer is typically a necessary step to further development of a useful product. The results

of the present process are thus at least as “useful, concrete and tangible” as the examples of acceptable processes given on page 2100-16 of the MPEP, and reconsideration of the examiner’s rejections is requested.

**35 U.S.C. § 112 ¶1:**

Claims 1-4 and 6-11 stand rejected on the ground that the specification does not provide enablement over the full scope of the claims.

The reference to “genetic engineering” on page 3 of the office action is believed to be erroneous because, as explained in a previous response, the present invention does not involve or relate to genetic engineering.

The examiner says that “specific and detailed guidance is required in order to carry out a modeling method to result in a molecular structure,” but does not clearly identify what he believes to be lacking from the guidance provided in the specification of the present application. The specification does identify how the invention in general is to be carried out. It is clear from the materials supplied with previous responses that computation using genetic algorithms is well known in general. See also the Library of Congress catalog, where the term “genetic algorithms” first appears as early as 1986. A patent need not teach, and preferably omits, what is well known in the art. *In re Buchner*, 929 F.2d 660, 661, 18 USPQ2d 1331,1332 (Fed. Cir. 1991). It is necessary only to explain to the reader how the generally-known mathematics of genetic algorithms is to be adapted to the specific subject matter of the invention. The key to that is to identify the variables that are likely to be important in determining the crystal structure, which is fully discussed in the specification. See, for example, page 4, lines 20-24 and page 8, line 25 to page 9, line 10.

The examiner’s reliance on Wormington does not assist the examiner. Wormington was issued with claims that are, in material respects, broader than those of the present invention, and are supported by only a single example. The Office has thus admitted that in this field a broad claim can be sufficiently enabled by a single example. The specific passage in Wormington cited by the examiner merely describes the problem underlying both

the present invention and Wormington, a problem which both Wormington and the present invention solve by a process of iterative alteration and selection. The examiner has not raised any new question of enablement that the Office has not already determined in the applicants' favor by issuing Wormington.

In view of the foregoing, reconsideration of this rejection is respectfully requested.

***35 U.S.C. § 112 ¶2:***

Claim 5 stands rejected on the ground that the Miller indices h and k are not defined. It is respectfully pointed out that the Miller indices are part of the normal vocabulary of persons skilled in the crystallographic arts, as is evidenced by the secondary materials accompanying applicants' responses to previous office actions, so that an explicit definition is totally unnecessary.

The notation used in the definitions of the components of I and F in claim 5 has been changed as requested by the examiner. A corresponding amendment has been made on pages 4 and 11.

Claims 8 and 9 have been amended to state explicitly that the unit cell and space group determined in claim 8, and the internal coordinates determined in claim 9, are those used as inputs at claim 1, lines 5 and 10.

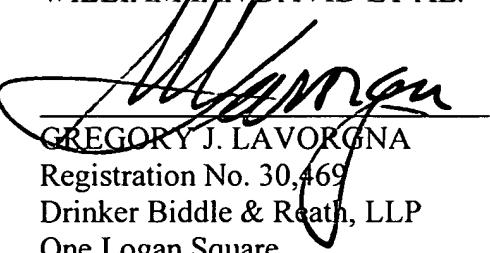
Claim 10 has been amended to explain explicitly that the process halts after the predetermined number of iterations if it has not already terminated by reaching the fitness threshold of claim 1.

***Conclusion:***

In view of the foregoing, reconsideration of the examiner's objections and rejections and an early notice of allowance of claims 1-11 are earnestly solicited.

Respectfully submitted,

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